

Dibromomethane
74-95-3 | DTXSID4021557

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.83e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.90e-01

Confidence level: 8.31e-01

Nearest Neighbors from the Training Set

Image not found

Dibromomethane

Measured: 6.85e-02

Predicted: 4.83e-02

Image not found

1,2-Dibromoethane

Measured: 2.21e-02

Predicted: 1.94e-02

Image not found

Ethane, iodo-

Measured: 2.51e-02

Predicted: 2.23e-02

Image not found

Methyl iodide

Measured: 9.72e-02

Predicted: 7.27e-02

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1,3-Cyclopentadiene

Measured: 2.72e-02

Predicted: 2.15e-02